

What is claimed is:

1. A method for optimizing crystallizing of a target molecule using a synthesizer and a computer, the method including the steps of:

5 identifying variables which affect crystallization;
choosing a finite number of experimental tests, wherein the experimental tests have values for the variables;

providing a plurality of wells;

assigning each of the experimental tests to a particular well;

10 dispensing reagents and solvents into a plurality of wells chosen from the values for the experimental tests;

crystallizing in the synthesizer using operating conditions chosen from the values for the experimental tests;

analyzing crystals in the plurality of the wells;

15 automatically generating a statistical analysis using the computer based on the analysis of the crystals in the plurality of the wells and at least one of the variables identified in order to evaluate the crystallization in the wells; and

automatically generating, using the computer, suggested parameters for future experiments based on the statistical analysis.

20 2. The method as claimed in claim 1 wherein the variables include temperature.

3. The method as claimed in claim 1 wherein the variables include reagent concentrations.

25 4. The method as claimed in claim 1 wherein one of the variables includes choice of solvents.

30 5. The method as claimed in claim 1 wherein one of the variables includes crystallization time.

6. The method as claimed in claim 1 wherein one of the variables includes crystallization partners.

7. The method as claimed in claim 1 wherein one of the variables includes concentration of at least one crystallization partner.

8. The method as claimed in claim 1 wherein one of the variables includes concentration of the target molecule.

9. The method as claimed in claim 1 wherein the step of choosing a finite number of experimental tests includes randomly choosing values for the variables from the range of values.

10. The method as claimed in claim 1 wherein the step of analyzing the samples includes determining whether crystals are formed.

11. The method as claimed in claim 1 wherein the step of analyzing the samples includes determining quantities of crystallized target compound formed in the wells.

12. The method as claimed in claim 1 wherein the step of analyzing the samples includes determining yields of crystallized target compound.

13. The method as claimed in claim 1 wherein the step of analyzing the samples includes determining the quality of the crystals formed.

14. The method as claimed in claim 13 wherein the step of determining the quality of the crystals formed includes determining the size of the crystals formed.

15. The method as claimed in claim 13 wherein the step of determining the quality of the crystals formed includes determining the color of the crystals formed.

16. The method as claimed in claim 13 wherein the step of determining the quality of the crystals formed includes visually inspecting the crystals.

5 17. The method as claimed in claim 13 wherein the step of determining the quality of the crystals formed includes analyzing the components of the crystals.

18. The method as claimed in claim 17 wherein the step of analyzing the components of the crystals includes analyzing for compounds other than the target
10 compound.

19. The method as claimed in claim 12 wherein the step of automatically generating a statistical analysis includes determining a most favorable crystallization in one of the plurality of wells based on the yields of crystallized target compound.
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20. The method as claimed in claim 1 wherein the step of automatically generating a statistical analysis includes graphically describing crystallizations based on the analysis of the crystals in the plurality of the wells.

20 21. The method as claimed in claim 15 wherein graphically describing the crystallizations includes generating multivariable contour maps.

22. A method for optimizing crystallizing of a target molecule using a synthesizer and a computer, the method including the steps of:

25 identifying variables which affect crystallization;
determining a range of values of the variables;
choosing a finite number of experimental tests, wherein the experimental tests have values for the variables chosen from the range of values;
providing a plurality of wells;
30 assigning each of the experimental tests to a particular well;

dispensing reagents and solvents into a plurality of wells chosen from the values for the experimental tests;

crystallizing in the synthesizer using operating conditions chosen from the values for the experimental tests;

5 analyzing crystals in the plurality of the wells;

automatically generating a statistical analysis using the computer based on the analysis of the crystals in the plurality of the wells and at least one of the variables identified in order to evaluate the crystallizations in the wells; and

10 automatically generating suggested parameters for future experiments using the computer wherein the suggested parameters are chosen from a new range of values based on the statistical analysis in order to optimize crystallization, the new range of values being different from the range of values.

15 23. The method as claimed in claim 22 wherein the new range of values is narrower than the range of values.

24. The method as claimed in claim 22 wherein the values for the experimental tests are chosen randomly from the range of values.

20 25. The method as claimed in claim 22 wherein the new range of values is narrower than the range of values.

26. A method for optimizing chiral resolution using a synthesizer, an analyzer and a computer, the method including the steps of:

25 identifying variables which affect chiral resolution;

choosing a finite number of experimental tests, wherein the experimental tests have values for the variables;

providing a plurality of wells;

assigning each of the experimental tests to a particular well;

30 dispensing reagents and solvents into a plurality of wells chosen from the values for the experimental tests;

crystallizing in the synthesizer using operating conditions chosen from the values for the experimental tests;

obtaining at least a portion of contents from the plurality of wells;

analyzing to determine the magnitude of chiral resolution for the at least a portion of the contents from the plurality of wells;

automatically generating a statistical analysis using the computer based on the step of determining the magnitude of chiral resolution and at least one of the variables identified in order to evaluate the chiral resolution in the wells; and

automatically generating, using the computer, suggested parameters for future experiments based on the statistical analysis.

27. The method of claim 26 wherein the step of analyzing to determine the magnitude of chiral resolution includes determining optical rotation of the at least a portion of the contents from the plurality of wells.

28. The method of claim 27 wherein the analyzer is a polarimeter.

29. The method of claim 27 wherein the analyzer is a chiral HPLC.

30. The method as claimed in claim 26 wherein one of the variables includes choice of solvents.

31. The method as claimed in claim 26 wherein one of the variables includes choice of crystallization partners.

32. The method as claimed in claim 26 wherein one of the variables includes concentration of at least one crystallization partner.